

=> fil lreg

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STRUCTURE FILE UPDATES: 14 OCT 2004 HIGHEST RN 762927-58-2
DICTIONARY FILE UPDATES: 14 OCT 2004 HIGHEST RN 762927-58-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
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=> fil hcap

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FILE COVERS 1907 - 15 Oct 2004 VOL 141 ISS 17
FILE LAST UPDATED: 14 Oct 2004 (20041014/ED)

This file contains CAS Registry Numbers for easy and accurate
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=> fil casreact

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FILE CONTENT:1840 - 10 Oct 2004 VOL 141 ISS 15

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*****
*
*   CASREACT now has more than  8 million reactions   *
*
*****
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil caold

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

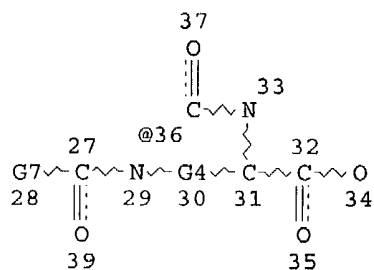
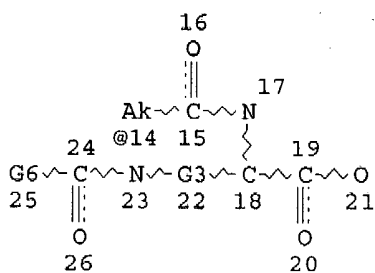
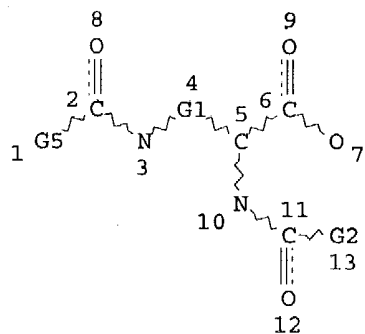
This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 15:30:39 ON 15 OCT 2004
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LAST RELOADED: Oct 8, 2004 (20041008/UP).

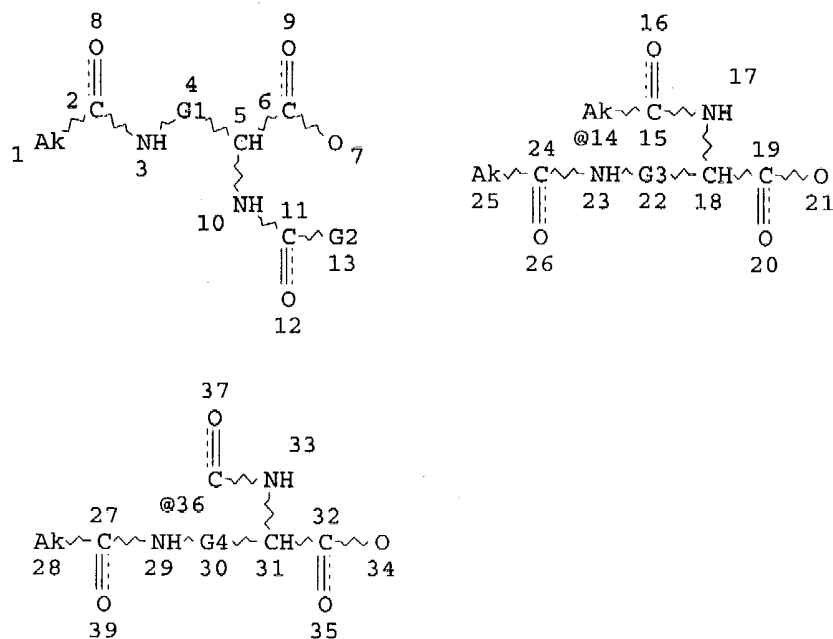
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L10 STR



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 REP G3=(1-6) C
 REP G4=(1-6) C
 VAR G5=CB/AK
 VAR G6=CB/AK
 VAR G7=CB/AK
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 NSPEC IS RC AT 7
 NSPEC IS RC AT 21
 NSPEC IS RC AT 34
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE
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 L17 STR



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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

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=> d l21

L21 ANALYZE L19 1- LC : 4 TERMS

TERM #	# OCC	# DOC	% DOC	LC
1	30	30	96.77	CA
2	30	30	96.77	CAPLUS
3	7	7	22.58	CASREACT
4	2	2	6.45	CAOLD

***** END OF L21***

=> d que nos l20

L10 STR
 L12 41 SEA FILE=REGISTRY SSS FUL L10
 L17 STR
 L19 31 SEA FILE=REGISTRY SUB=L12 SSS FUL L17
 L20 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L19

=> d que nos l22

L10 STR
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L17 STR
L19 31 SEA FILE=REGISTRY SUB=L12 SSS FUL L17
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=> d que nos l23

L10 STR
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L17 STR
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L23 1 SEA FILE=CAOLD ABB=ON PLU=ON L19

=> dup rem l20 l22 l23

DUPLICATE IS NOT AVAILABLE IN 'CAOLD'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE

FILE 'HCAPLUS' ENTERED AT 15:31:12 ON 15 OCT 2004
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PROCESSING COMPLETED FOR L20
PROCESSING COMPLETED FOR L22
PROCESSING COMPLETED FOR L23

L24 6 DUP REM L20 L22 L23 (1 DUPLICATE REMOVED)
ANSWERS '1-5' FROM FILE HCAPLUS
ANSWER '6' FROM FILE CAOLD

=> d iall hitstr 1-5

L24 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2003:627026 HCAPLUS
DOCUMENT NUMBER: 139:337687
ENTRY DATE: Entered STN: 15 Aug 2003
TITLE: New gemini organogelators linked by oxalyl amide:
organogel formation and their thermal stabilities
AUTHOR(S): Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko;
Kimura, Mutsumi; Shirai, Hirofusa; Hanabusa, Kenji
CORPORATE SOURCE: Graduate School of Science and Technology, Shinshu
University, Ueda, Nagano, 386-8567, Japan
SOURCE: Tetrahedron Letters (2003), 44(36), 6841-6843
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 22-10 (Physical Organic Chemistry)

Section cross-reference(s): 34, 66, 77

OTHER SOURCE(S): CASREACT 139:337687

ABSTRACT:

New gemini organogelators linked by an oxalyl amide that can be easily, effectively, and cheaply synthesized have good organogelation abilities and their cyclohexane gels have superior thermal stabilities; especially 7 possessing the branched alkyl ester can gel at 0.7 wt% cyclohexane even at 70°C.

SUPPL. TERM: gemini organogelator oxalylamide organogel formation thermal stability

INDEX TERM: Gelation
Hydrogen bond
Sol-gel processing
Solvents
Thermal stability
(NMR and FT-IR on gelation of prepared gemini oxalyl-amide linked organogelators)INDEX TERM: Gelation agents
(organo; NMR and FT-IR on gelation of prepared gemini oxalyl-amide linked organogelators)INDEX TERM: 615584-80-0P 615584-81-1P
615584-82-2P 615584-83-3P
615584-84-4P 615584-85-5P
615584-86-6P

ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(NMR and FT-IR on gelation of prepared gemini oxalyl-amide linked organogelators)

INDEX TERM: 52315-75-0, N-Lauroyl-L-lysine 292140-08-0 340811-55-4
521974-57-2 615584-87-7 615584-88-8 615584-89-9

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(NMR and FT-IR on gelation of prepared gemini oxalyl-amide linked organogelators)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD.

- REFERENCE(S):
- (1) Ajayaghosh, A; J Am Chem Soc 2001, V123, P5148 HCAPLUS
 - (2) Becerril, J; Chem Commun 2002, P738 HCAPLUS
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HCAPLUS

- (24) Ono, Y; Chem Commun 1998, P1477 HCAPLUS
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 (27) Shumburo, A; Chem Mater 2002, V14, P3745 HCAPLUS
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 (35) Wang, G; Chem Eur J 2002, V8, P1954 HCAPLUS
 (36) Willemen, H; Eur J Org Chem 2001, P2329 HCAPLUS

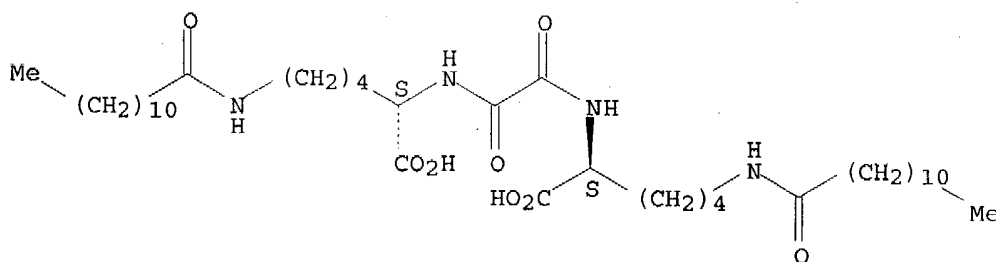
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 615584-83-3P 615584-84-4P 615584-85-5P
 615584-86-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (NMR and FT-IR on gelation of prepared gemini oxalyl-amide linked
 organogelators)

RN 615584-80-0 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)- (9CI)
 (CA INDEX NAME)

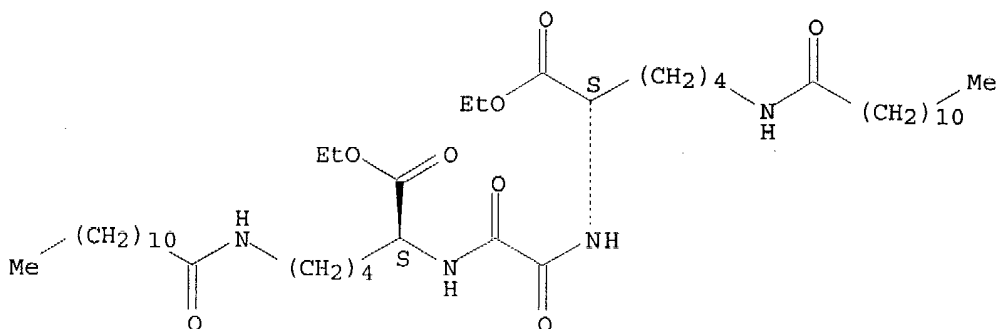
Absolute stereochemistry.



RN 615584-81-1 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, diethyl
 ester (9CI) (CA INDEX NAME)

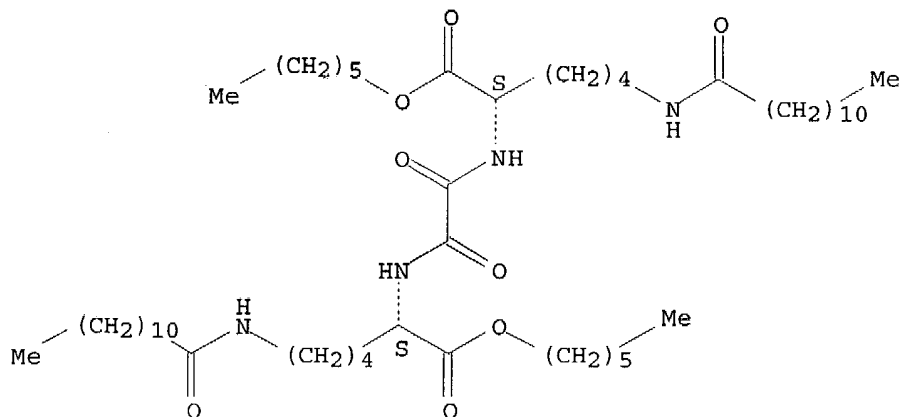
Absolute stereochemistry.



RN 615584-82-2 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, dihexyl ester (9CI) (CA INDEX NAME)

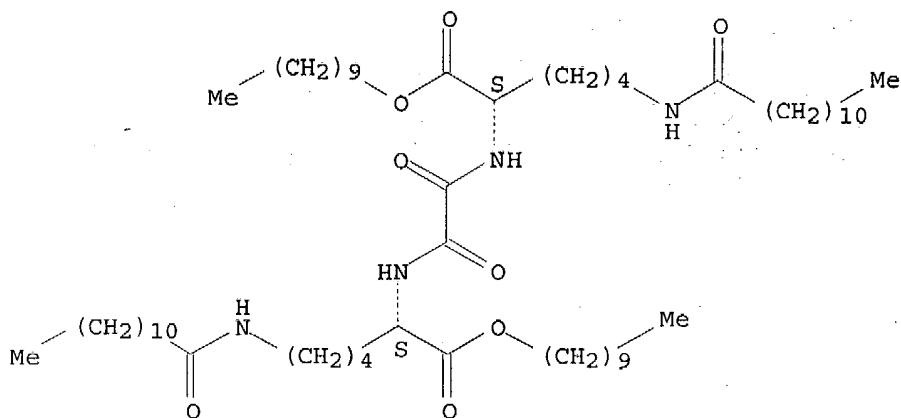
Absolute stereochemistry.



RN 615584-83-3 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, didecyl ester (9CI) (CA INDEX NAME)

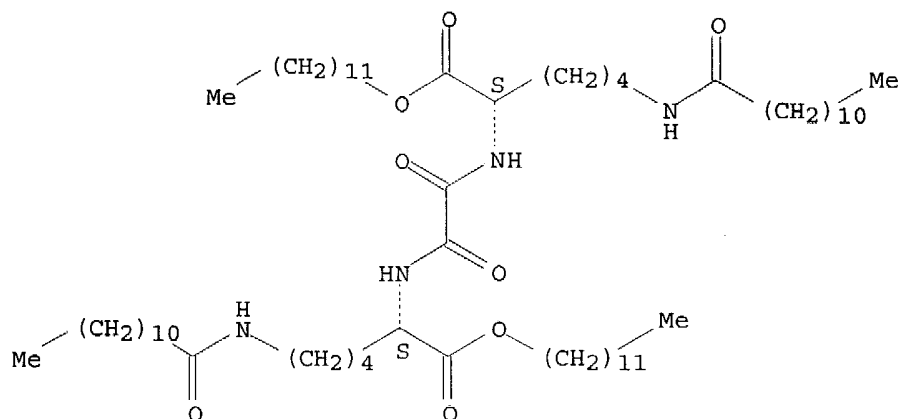
Absolute stereochemistry.



RN 615584-84-4 HCAPLUS

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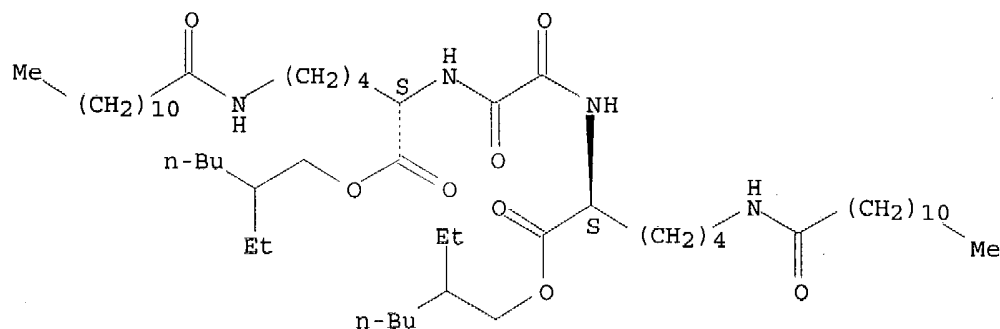
Absolute stereochemistry.



RN 615584-85-5 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

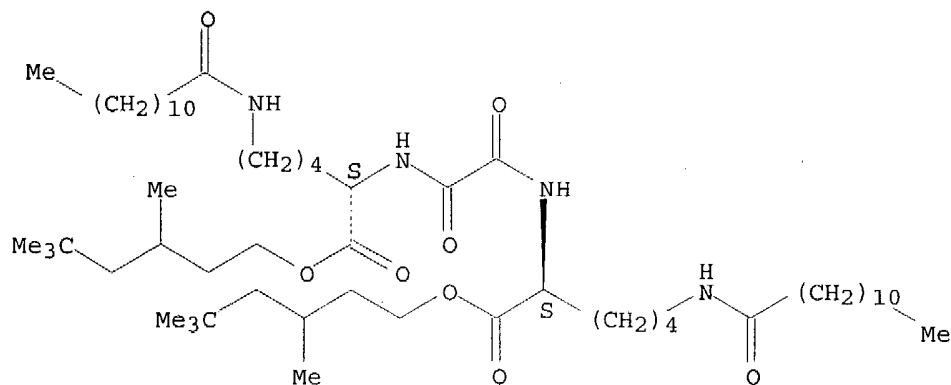
Absolute stereochemistry.



RN 615584-86-6 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, bis(3,5,5-trimethylhexyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:878000 HCAPLUS

DOCUMENT NUMBER: 140:181736

ENTRY DATE: Entered STN: 10 Nov 2003

TITLE: L-Lysine based gemini organogelators: their organogelation properties and thermally stable organogels

AUTHOR(S): Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko;

Kimura, Mutsumi; Shirai, Hirofusa; Hanabusa, Kenji

CORPORATE SOURCE: Graduate School of Science and Technology, Shinshu

University, Ueda, Nagano, 386-8567, Japan

SOURCE: Organic & Biomolecular Chemistry (2003), 1(22), 4124-4131

CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 34-2 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 66

ABSTRACT:

Novel gemini organogelators based on L-lysine, in which two L-lysine derivs. are linked by different alkylene chain lengths through the amide bond, have been simply and effectively synthesized, and their organogelation abilities and thermal stabilities have been investigated. In a series of L-lysine Et ester derivs., the organogelation abilities decreased with increasing alkylene spacer length. In particular, bis(Nε-lauroyl-L-lysine Et ester)oxalyl amide, H₂3C11CONH(CH₂)₄CH(CO₂Et)NH-COCO-NHCH(CH₂)₄NHCOC11H₂₃, is a good organogelator that gels most organic solvents such as alcs., cyclic ethers, aromatic solvents and acetonitrile. Various oxalyl amide derivs. with different alkyl ester groups such as hexyl, decyl, dodecyl, 2-ethyl-1-hexyl and 3,5,5-trimethylhexyl also showed good organogelation abilities. Furthermore, it was found that the cyclohexane gels formed by some oxalyl amide derivs. have a high thermal stability.

SUPPL. TERM: lysine bis amide alkylene prepn organogelator thermal stability

INDEX TERM: Solvent effect
(effects of organic solvents on organogelation properties of bis-lysine amides linked by alkylene chains)INDEX TERM: Molecular structure-property relationship
(gelation; preparation, organogelation property and thermal stability of bis-lysine amides linked by alkylene chains)INDEX TERM: Gelation
Gelation agents
Thermal stability
(preparation, organogelation property and thermal stability of bis-lysine amides linked by alkylene chains)INDEX TERM: 615584-80-0P 615584-81-1P
615584-82-2P 615584-83-3P
615584-84-4P 615584-85-5P
615584-86-6P 658051-84-4P
658051-85-5P 658051-86-6P
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658051-99-1P 658052-00-7P

658052-01-8P

ROLE: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation, organogelation property and thermal stability of bis-lysine amides linked by alkylene chains)

INDEX TERM: 79-37-8, Oxalyl chloride 111-19-3, Sebacoyl chloride 111-27-3, n-Hexanol, reactions 111-50-2, Adipoyl chloride 112-16-3, Lauroyl chloride 112-30-1, 1-Decanol 112-53-8, Dodecyl alcohol 123-98-8, Azelaoyl chloride 142-79-0, Pimeloyl chloride 543-20-4, Succinyl chloride 1663-67-8, Malonyl chloride 2873-74-7, Glutaryl chloride 3452-97-9, 3,5,5-Trimethylhexanol 4834-98-4, Dodecanedioyl dichloride 10027-07-3, Suberoyl chloride 52315-75-0

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(preparation, organogelation property and thermal stability of bis-lysine amides linked by alkylene chains)

INDEX TERM: 340811-55-4P 521974-57-2P 614723-86-3P 615584-87-7P 615584-88-8P 615584-89-9P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, organogelation property and thermal stability of bis-lysine amides linked by alkylene chains)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD.

- REFERENCE(S):
- (1) Ajayaghosh, A; J Am Chem Soc 2001, V123, P5148 HCAPLUS
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 - (3) de Loos, M; Angew Chem, Int Ed 2001, V40, P613 HCAPLUS
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 - (30) Terech, P; Chem Rev 1997, V97, P3133 HCAPLUS
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 - (32) van Bommel, K; Angew Chem, Int Ed 2003, V42, P980 HCAPLUS
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 (35) van der Laan, S; Langmuir 2002, V18, P7136 HCAPLUS
 (36) Velasco-Garcia, N; Analyst 1997, V122, P5008
 (37) Wang, G; Chem Eur J 2002, V8, P1954 HCAPLUS
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 (39) Willemen, H; Eur J Org Chem 2001, P2329 HCAPLUS
 (40) Yamada, N; Langmuir 2001, V17, P961 HCAPLUS

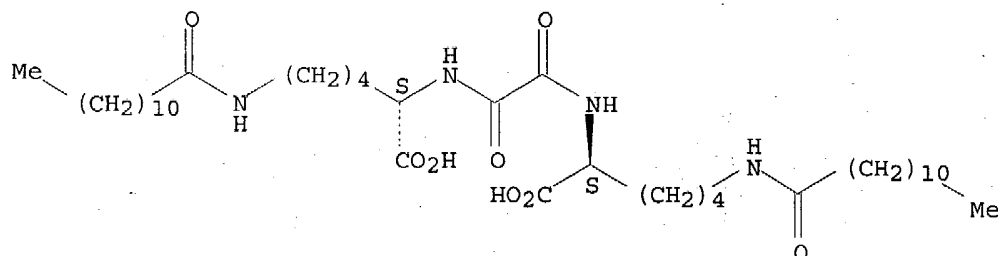
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 658052-01-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation, organogelation property and thermal stability of bis-lysine
 amides linked by alkylene chains)

RN 615584-80-0 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)- (9CI)
 (CA INDEX NAME)

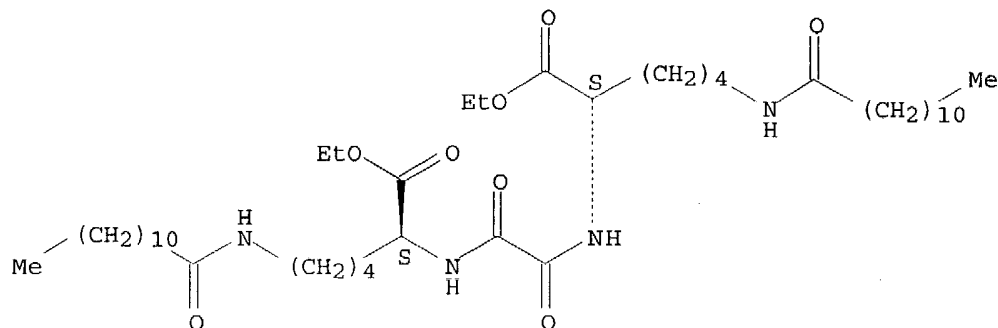
Absolute stereochemistry.



RN 615584-81-1 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, diethyl
 ester (9CI) (CA INDEX NAME)

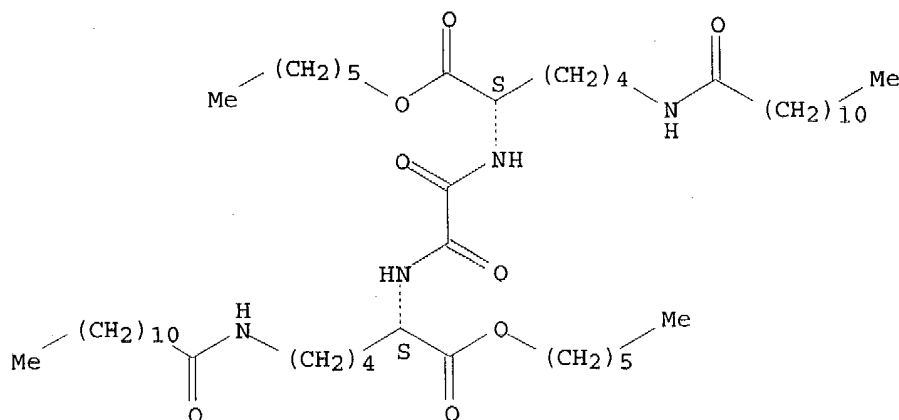
Absolute stereochemistry.



RN 615584-82-2 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, dihexyl
 ester (9CI) (CA INDEX NAME)

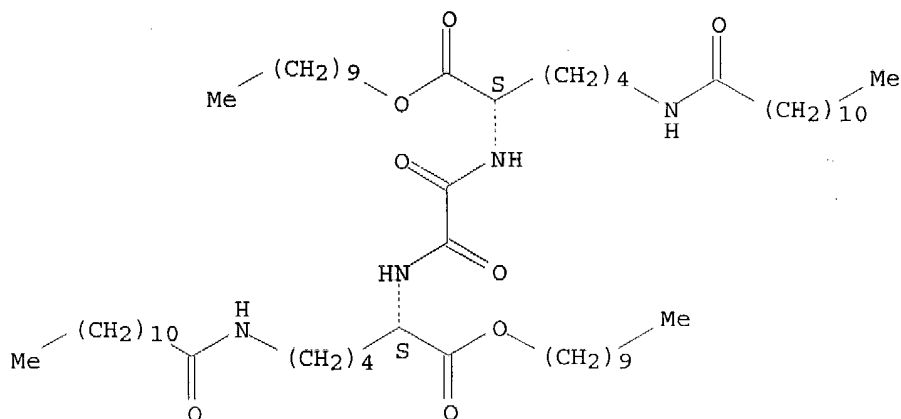
Absolute stereochemistry.



RN 615584-83-3 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, didecyl ester (9CI) (CA INDEX NAME)

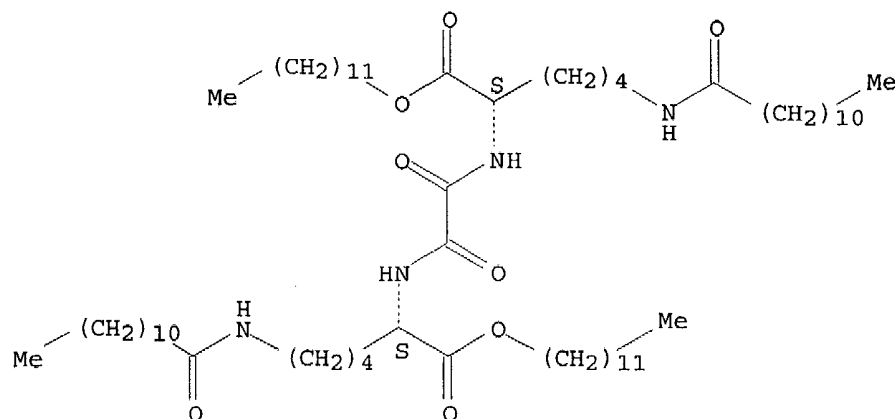
Absolute stereochemistry.



RN 615584-84-4 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, didodecyl ester (9CI) (CA INDEX NAME)

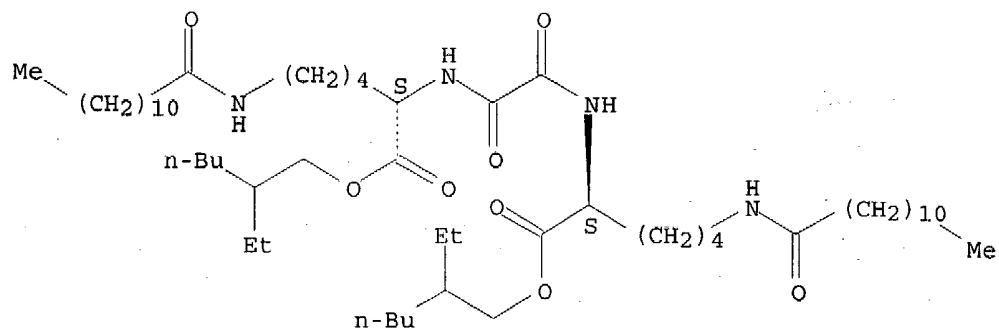
Absolute stereochemistry.



RN 615584-85-5 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

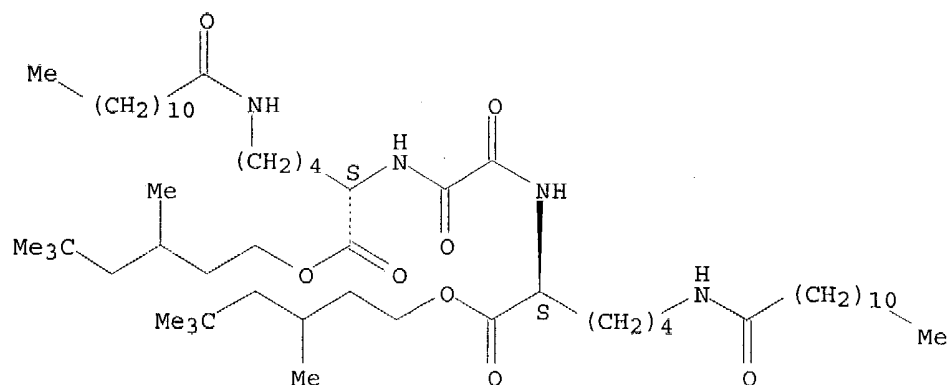
Absolute stereochemistry.



RN 615584-86-6 HCAPLUS

CN L-Lysine, N2,N2'-(1,2-dioxo-1,2-ethanediyl)bis[N6-(1-oxododecyl)-, bis(3,5,5-trimethylhexyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

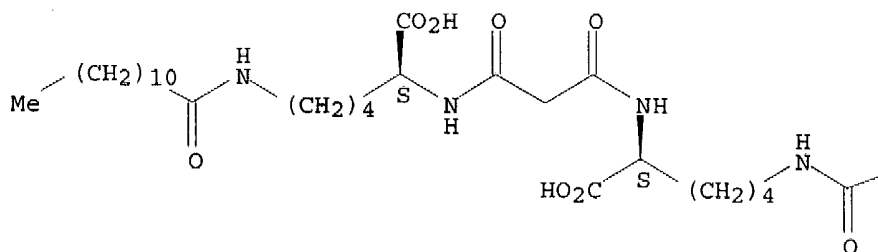


RN 658051-84-4 HCAPLUS

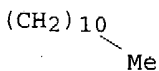
CN L-Lysine, N2,N2'-(1,3-dioxo-1,3-propanediyl)bis[N6-(1-oxododecyl) - (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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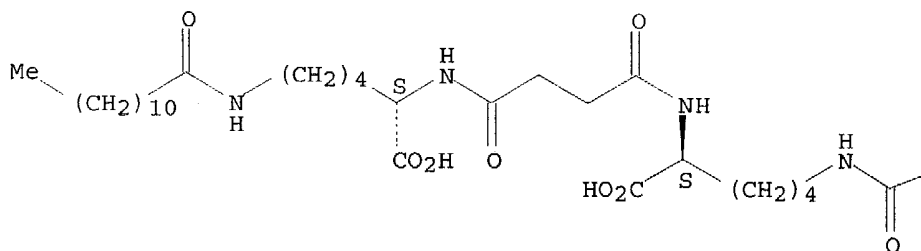


RN 658051-85-5 HCAPLUS

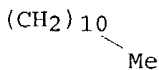
CN L-Lysine, N2,N2'-(1,4-dioxo-1,4-butanediyl)bis[N6-(1-oxododecyl) - (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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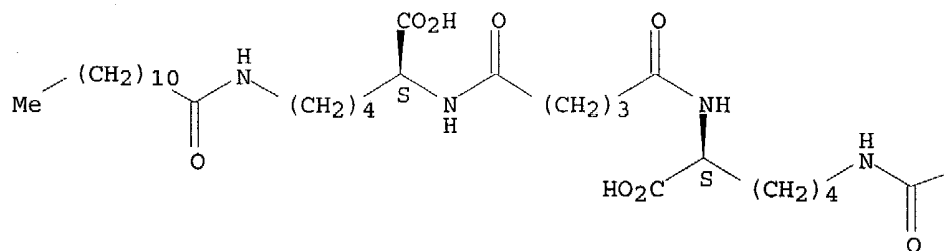


RN 658051-86-6 HCAPLUS

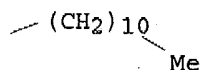
CN L-Lysine, N2,N2'-(1,5-dioxo-1,5-pentanediy1)bis[N6-(1-oxododecyl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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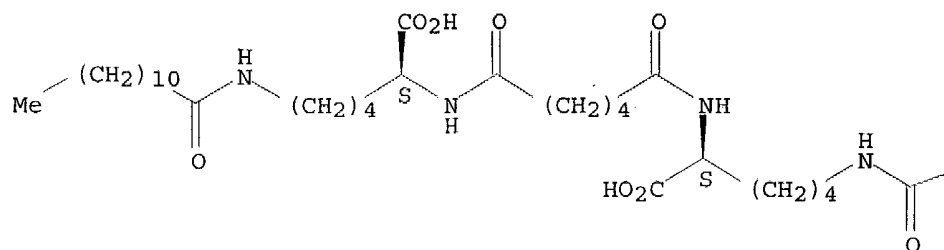


RN 658051-87-7 HCAPLUS

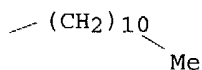
CN L-Lysine, N2,N2'-(1,6-dioxo-1,6-hexanediy1)bis[N6-(1-oxododecyl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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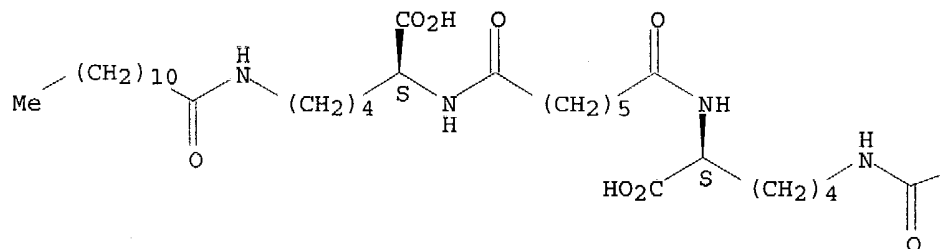


RN 658051-88-8 HCAPLUS

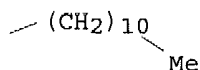
CN L-Lysine, N2,N2'-(1,7-dioxo-1,7-heptanediyl)bis[N6-(1-oxododecyl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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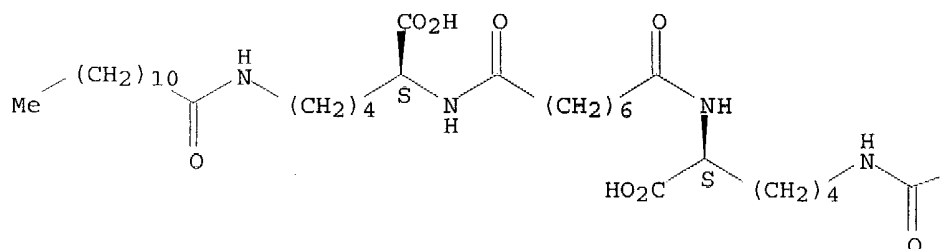


RN 658051-89-9 HCAPLUS

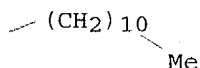
CN L-Lysine, N2,N2'-(1,8-dioxo-1,8-octanediyl)bis[N6-(1-oxododecyl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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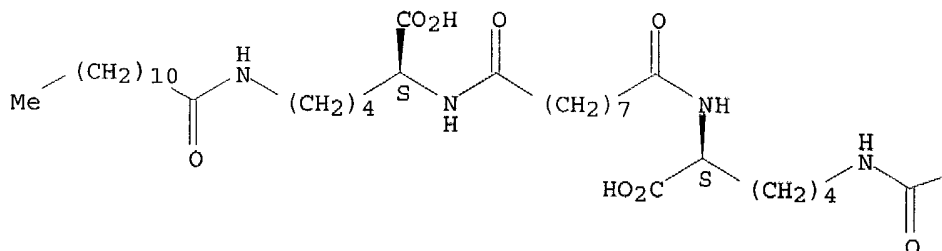


RN 658051-90-2 HCAPLUS

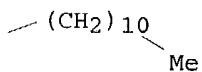
CN L-Lysine, N2,N2'-(1,9-dioxo-1,9-nonanediyl)bis[N6-(1-oxododecyl) - (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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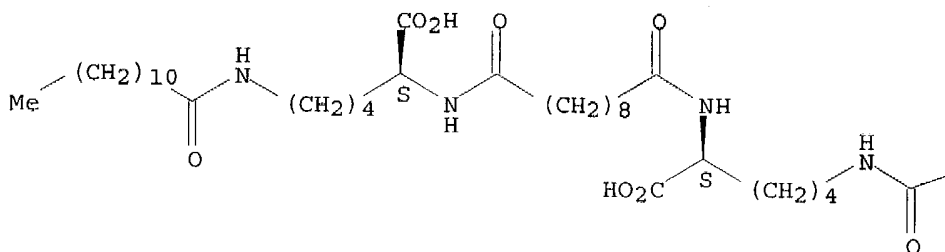


RN 658051-91-3 HCAPLUS

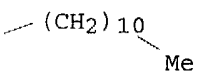
CN L-Lysine, N2,N2'-(1,10-dioxo-1,10-decanediyl)bis[N6-(1-oxododecyl) - (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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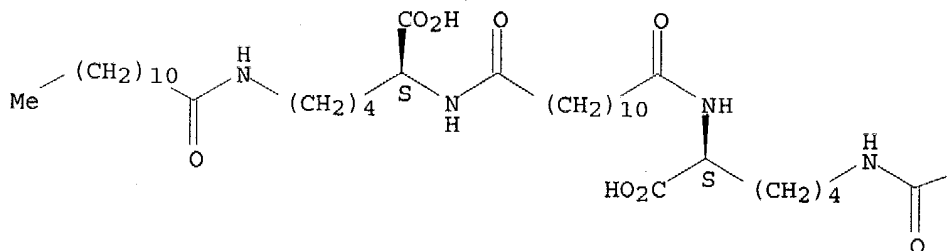


RN 658051-92-4 HCAPLUS

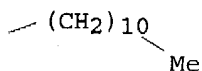
CN L-Lysine, N2,N2'-(1,12-dioxo-1,12-dodecanediyl)bis[N6-(1-oxododecyl)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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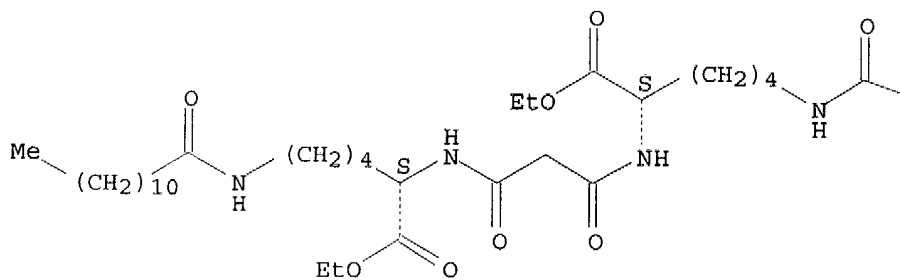


RN 658051-93-5 HCAPLUS

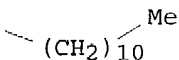
CN L-Lysine, N2,N2'-(1,3-dioxo-1,3-propanediyl)bis[N6-(1-oxododecyl)-,
diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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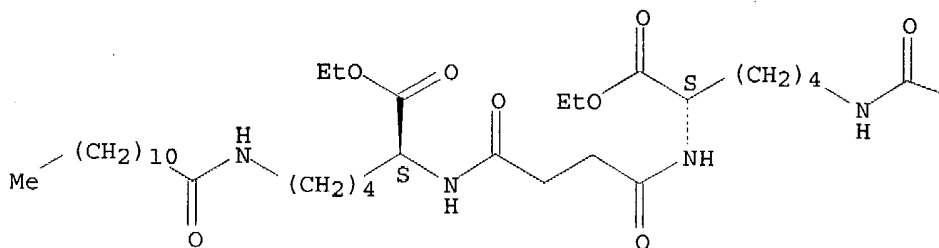


RN 658051-94-6 HCAPLUS

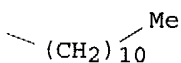
CN L-Lysine, N2,N2'-(1,4-dioxo-1,4-butanediyl)bis[N6-(1-oxododecyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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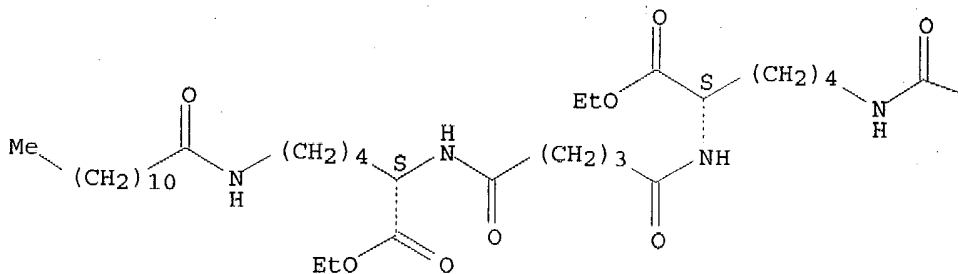


RN 658051-95-7 HCAPLUS

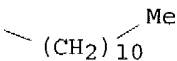
CN L-Lysine, N2,N2'-(1,5-dioxo-1,5-pentanediy)bis[N6-(1-oxododecyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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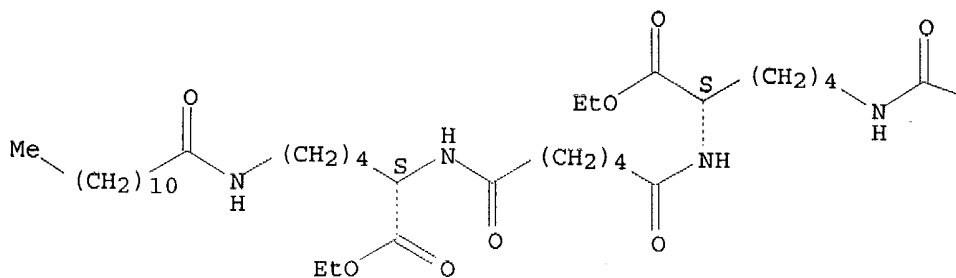


RN 658051-96-8 HCAPLUS

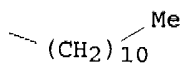
CN L-Lysine, N2,N2'-(1,6-dioxo-1,6-hexanediy)bis[N6-(1-oxododecyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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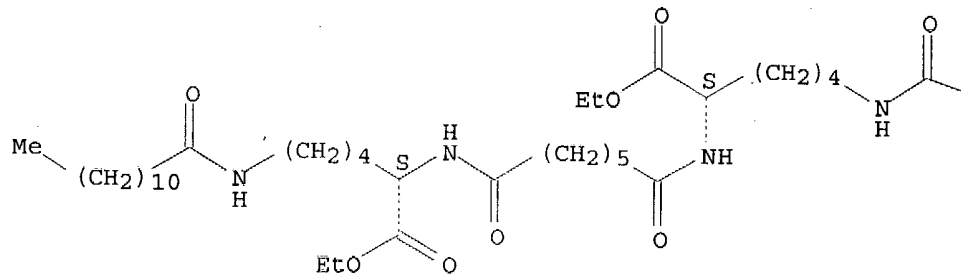


RN 658051-97-9 HCAPLUS

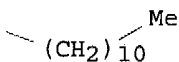
CN L-Lysine, N2,N2'-(1,7-dioxo-1,7-heptanediyl)bis[N6-(1-oxododecyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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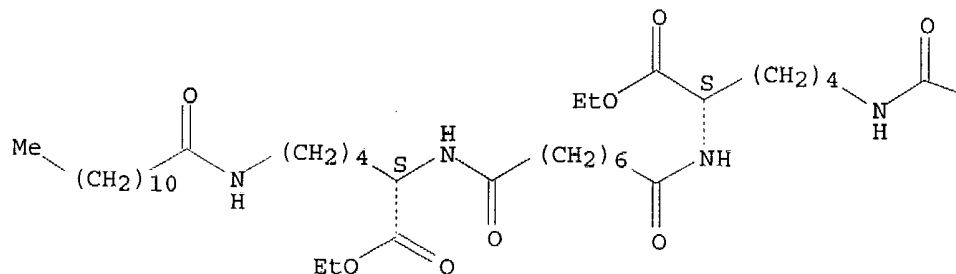


RN 658051-98-0 HCAPLUS

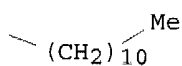
CN L-Lysine, N2,N2'-(1,8-dioxo-1,8-octanediyl)bis[N6-(1-oxododecyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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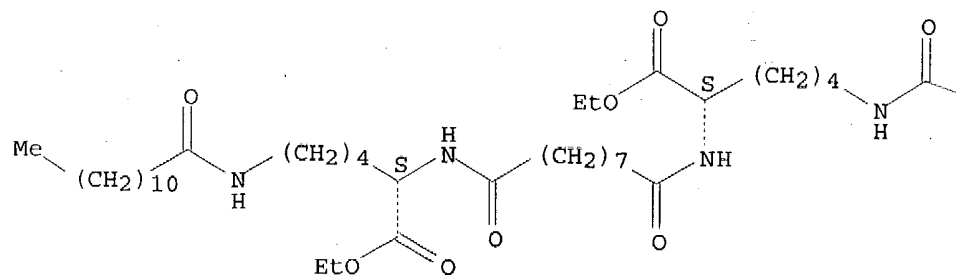


RN 658051-99-1 HCAPLUS

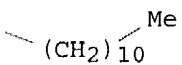
CN L-Lysine, N2,N2'-(1,9-dioxo-1,9-nonanediyloxybis[N6-(1-oxododecyl)-], diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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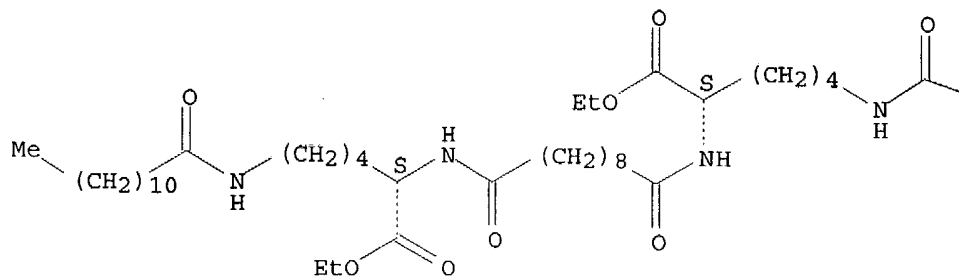


RN 658052-00-7 HCAPLUS

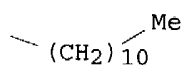
CN L-Lysine, N2,N2'-(1,10-dioxo-1,10-decanediyl)bis[N6-(1-oxododecyl)-], diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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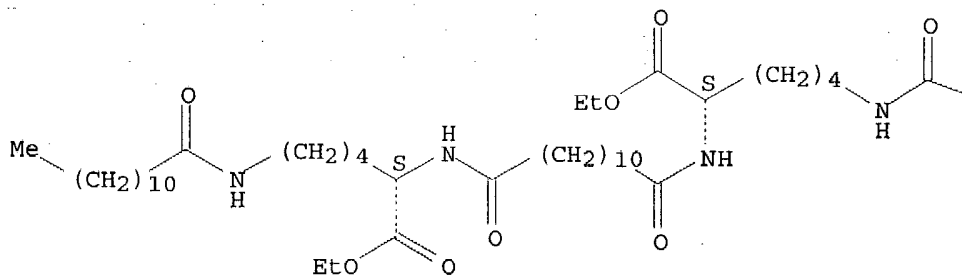


RN 658052-01-8 HCAPLUS

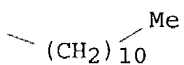
CN L-Lysine, N2,N2'-(1,12-dioxo-1,12-dodecanediyl)bis[N6-(1-oxododecyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L24 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:334995 HCAPLUS

DOCUMENT NUMBER: 127:51064

ENTRY DATE: Entered STN: 26 May 1997

TITLE: Synthesis and characterization of random and regular L-lysine-based polyamides

AUTHOR(S): Gachard, Isabelle; Coutin, Bernard; Sekiguchi, Hikaru

CORPORATE SOURCE: Laboratoire Chimie Macromoleculaire, Universitet

SOURCE: Pierre et Marie Curie, Paris, F-75252, Fr.
Macromolecular Chemistry and Physics (1997), 198(5),
1375-1389
CODEN: MCHPES; ISSN: 1022-1352

PUBLISHER: Huethig & Wepf

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 35-5 (Chemistry of Synthetic High Polymers)

ABSTRACT:
The synthesis of polyamides based on the natural diamine L-lysine and diacids, adipic or glutaric acid, is described. They were obtained by polycondensation of active diesters, pentachlorophenyl, and pentafluorophenyl esters. L-Lysine being non-sym., aregular (random), and syndioregular (head-to-head, tail-to-tail) poly(adipoyl-L-lysine)s and poly(glutaroyl-L-lysine)s were obtained with mol. wts. > 15,000 while isoregular (head-to-tail) poly(adipoyl-L-lysine)s and poly(glutaroyl-L-lysine)s were prepared with lower mol. wts.

SUPPL. TERM: amino diacid lysine polymer syndioregular prepn; polyamide
lysine adipic glutaric syndioregular prepn

INDEX TERM: Polyamides, preparation
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)
(preparation and characterization of random and regular
L-lysine-based polyamides with adipic or glutaric acid)

INDEX TERM: 191230-54-3P 191230-57-6P
ROLE: PRP (Properties); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; preparation and characterization of random and
regular L-lysine-based polyamides with adipic or glutaric
acid)

INDEX TERM: 6366-70-7P 191230-53-2P 191230-55-4P 191230-56-5P
ROLE: PRP (Properties); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and characterization of random and regular
L-lysine-based polyamides with adipic or glutaric acid)

INDEX TERM: 191230-58-7P 191230-59-8P 191230-60-1P 191230-61-2P
191230-62-3P 191230-63-4P 191230-64-5P
191230-65-6P 191230-66-7P 191230-68-9P 191230-69-0P
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)
(preparation and characterization of random and regular
L-lysine-based polyamides with adipic or glutaric acid)

INDEX TERM: 87-86-5, Pentachlorophenol 100-51-6, Benzyl alcohol,
reactions 405-39-0, N,N'-Bis(benzyloxycarbonyl)-L-lysine
2035-75-8, Adipic anhydride 10416-59-8,
N,O-Bis(trimethylsilyl)acetamide 16259-78-2 83701-40-0,
Hexanedioic acid, bis(pentafluorophenyl) ester
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation and characterization of random and regular
L-lysine-based polyamides with adipic or glutaric acid)

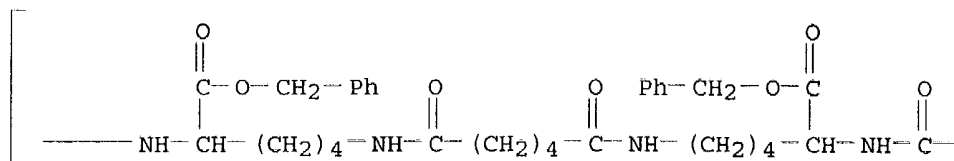
INDEX TERM: 191230-52-1P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of random and regular
L-lysine-based polyamides with adipic or glutaric acid)

IT 191230-62-3P 191230-64-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of random and regular L-lysine-based
polyamides with adipic or glutaric acid)

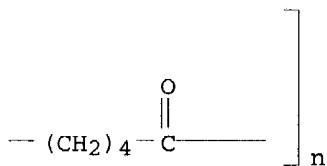
RN 191230-62-3 HCAPLUS

CN Poly[imino[1-[(phenylmethoxy)carbonyl]-1,5-pentanediy]imino(1,6-dioxo-1,6-hexanediy]imino[5-[(phenylmethoxy)carbonyl]-1,5-pentanediy]imino(1,6-dioxo-1,6-hexanediy)], [S-(R*,R*)] - (9CI) (CA INDEX NAME)

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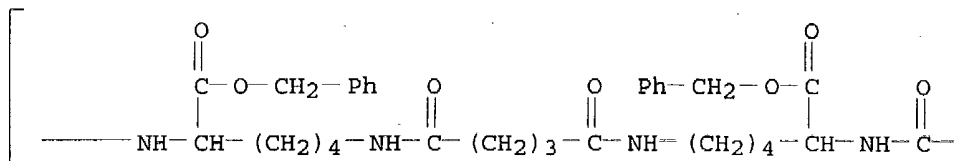
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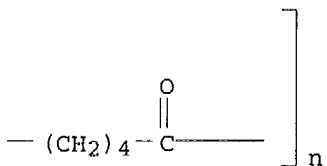
RN 191230-64-5 HCAPLUS

CN Poly[imino[(1S)-1-[(phenylmethoxy)carbonyl]-1,5-pentanediy]imino(1,5-dioxo-1,5-pentanediy]imino[(5S)-5-[(phenylmethoxy)carbonyl]-1,5-pentanediy]imino(1,6-dioxo-1,6-hexanediy)] (9CI) (CA INDEX NAME)

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L24 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1968:13536 HCAPLUS

DOCUMENT NUMBER: 68:13536

ENTRY DATE: Entered STN: 12 May 1984

TITLE: Optically active polyamides with regular structural sequences prepared from α -amino acids

AUTHOR(S): Saotome, Kazuo; Schulz, Rolf Christian
 CORPORATE SOURCE: Univ., Mainz, Mainz, Fed. Rep. Ger.
 SOURCE: Makromolekulare Chemie (1967), 109, 239-48
 CODEN: MACEAK; ISSN: 0025-116X

DOCUMENT TYPE: Journal
 LANGUAGE: English
 CLASSIFICATION: 35 (Synthetic High Polymers)

ABSTRACT:

Optically active polyamides with regular structural sequences were prepared from L-lysine and adipic acid. An optically active sym. diamine, N,N'-bis(L-5-amino-5-carboxy-1-aminopentyl) adipamide, m. 305° (decomposition), was obtained by treating L-lysine with adipoyl chloride (I) in the presence of Cu²⁺. The interfacial polycondensation of this diamine with I gave a regular polymer, while the polycondensation of L-lysine with I gave an irregular polymer of the same anal. composition. The m.ps., optical rotations, and the O.R.D. curves of these polymers were investigated.

SUPPL. TERM: POLYAMIDES OPTICALLY ACTIVE; OPTICALLY ACTIVE POLYAMIDES;
 ADIPIC ACID LYSINE POLYAMIDES; AMINO ACID POLYAMIDES;
 LYSINE-ADIPIC ACID POLYAMIDES

INDEX TERM: Chains, chemical
 (configuration or conformation of, of adipic acid-lysine
 polyamides, O.R.D. in relation to)

INDEX TERM: Polyamides, preparation
 ROLE: PREP (Preparation)
 (from adipic acid and lysine, O.R.D. in relation to chain
 configuration of)

INDEX TERM: Optical rotatory dispersion
 (of adipic acid-lysine polyamides, chain configuration in
 relation to)

INDEX TERM: 18784-13-9
 ROLE: USES (Uses)
 (model compound for adipic acid-lysine polyamides)

INDEX TERM: 18784-11-7P 18784-12-8P
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

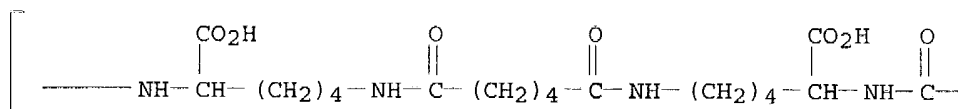
INDEX TERM: 26760-94-1P 29612-49-5P 29615-94-9P 29615-95-0P
 32029-32-6P 32032-03-4P
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, and O.R.D. in relation to chain configuration
 thereof)

IT 32029-32-6P 32032-03-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, and O.R.D. in relation to chain configuration thereof)

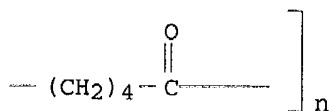
RN 32029-32-6 HCAPLUS

CN Poly[imino[(1S)-1-carboxy-1,5-pentanediy]imino(1,6-dioxo-1,6-
 hexanediyl)imino[(5S)-5-carboxy-1,5-pentanediy]imino(1,6-dioxo-1,6-
 hexanediyl)] (9CI) (CA INDEX NAME)

PAGE 1-A

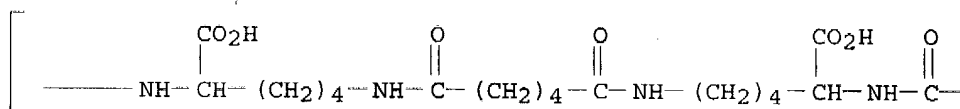


PAGE 1-B

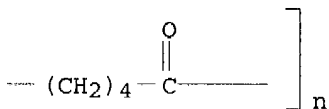


RN 32032-03-4 HCAPLUS
 CN Poly[imino[(1S)-1-carboxy-1,5-pentanediy]]imino(1,6-dioxo-1,6-hexanediyl)imino[(5S)-5-carboxy-1,5-pentanediy]]imino(1,6-dioxo-1,6-hexanediyl)], rel- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L24 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:3568 HCAPLUS

DOCUMENT NUMBER: 60:3568

ORIGINAL REFERENCE NO.: 60:657g-h, 658a-h, 659a-d

ENTRY DATE: Entered STN: 22 Apr 2001

TITLE: Peptides. XXXV. Synthesis of α , ω -oligamides from L-glutamic acid and L-lysine

AUTHOR(S): Zahn, Helmut; Paetzold, Walter

CORPORATE SOURCE: Tech. Hochschule, Aachen, Germany

SOURCE: Ber. (1963), 96(10), 2566-76

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

CLASSIFICATION: 44 (Amino Acids, Peptides, and Proteins)

OTHER SOURCE(S): CASREACT 60:3568

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

ABSTRACT:

cf. CA 59, 751g. Several oligamides of the nylon-5,5 type with alternately a free CO₂H and NH₂ monomer unit were prepared by the method of the peptide chemistry from glutamic acid and lysine derivs. Derivs. of these 2 amino acids were subjected to polycondensations. The decomposition of the various condensation products by boiling with H₂O and their behavior towards HNO₂ were investigated. PhCH₂O₂CCH(NHCO₂CH₂Ph)CH₂CH₂CO₂H (9.5 g.) in 80 cc. dry tetrahydrofuran treated 0.5 hr. at -10° with 3.5 cc. Et₃N and 2.4 cc. ClCO₂Et and then dropwise with 9.0 g. lysine-Cu complex-HCl and 7 cc. Et₃N in 50 cc. H₂O and 30 cc. tetrahydrofuran during 1 hr., stirred 2 hrs. with warming to 0°, poured with stirring into 0.75 l. iced H₂O, and filtered yielded 8.5 g. PhCH₂O₂CCH(NHCO₂CH₂Ph)CH₂CH₂CO-Lys-OH (I), m. 200° (decomposition) (EtOH). I

(4.8 g.) in 40 cc. H₂O and 10 cc. AcOH treated with stirring with 10% aqueous KCN until decolorized and refrigerated several hrs. yielded 4.4 g. N-carbobenzyloxy- α -benzyl- γ -Glu-Lys-OH.0.5H₂O (II), m. 204° (H₂O), Rf 0.85 (75:15:10 EtMeCHOH-90% HCO₂H-H₂O; solvent A); Rf 0.35 (85:15 EtMeCHOH-10% NH₄OH; solvent B). II (2.0 g.) in 50 cc. 90% tert-BuOH hydrogenated 2 hrs. over 50 mg. Pd black and the mixture filtered and evaporated yielded 1.1 g. N ϵ - γ -Glu-Lys-OH, powder, decomposed 250°, Rf 0.04 (A), 0.0 (B), 0.27 (free peptide) and 0.57 (HCl salt) (80% aqueous PhOH). Carbobenzyloxyglutamic acid (III) (10.3 g.) in 70 cc. MeCN treated with 17 g. dicyclohexylcarbodiimide (IV) in 30 cc. MeCN and then dropwise with 21.5 g. N ϵ -carbobenzyloxyllysine Et ester (V) in 40 cc. MeCN, kept at 0° overnight, and filtered, the residue boiled with EtOAc, and the combined filtrates treated with a little AcOH, filtered, and evaporated gave 24.8 g. VI (X and X' = PhCH₂O₂C) (VII), m. 113° (EtOAc), Rf 1.0 (A), 0.85 (B). VII (3 g.) in 150 cc. dry C₆H₆ treated 0.5 hr. at room temperature with dry HBr and refrigerated several hrs. gave VI.3HBr (X and X' = H) (VIII.3HBr) hygroscopic powder, Rf 0.09 (A), 0.28 (B). VIII.3HBr (about 1 g.) in 10 cc. acetate buffer (pH 4.6) treated with saturated aqueous Reinecke salt, heated to solution, and cooled deposited the trireineckate of VIII, pink powder, m. 150° (decomposition) (H₂O). Trifluoroacetylglutamic acid (IX) (4.8 g.) in 75 cc. MeCN, 9 g. IV in 25 cc. MeCN, and 19.3 g. V in 50 cc. MeCN refrigerated 5 days and filtered, the residue boiled with 300 cc. EtOAc and filtered off, and the viscous residue from the extract dissolved in 150 cc. warm EtOAc and kept 24 hrs. deposited 12.3 g. VI (X = CF₃CO, X' = H) (X), m. 135° with sintering, Rf 0.95 (A). IX (26 g.) in 300 cc. dry EtOAc treated with stirring with 27.8 g. p-O₂NC₆H₄OH and 41.2 g. IV, stirred 6 hrs., kept over-night, and worked up yielded 32 g. bis(p-nitrophenyl) ester (XI) of IX, needles, m. 144° (C₆H₆). XI (9.7 g.) in 50 cc. dry EtOAc treated dropwise at 0° with stirring with 12.3 g. V in 50 cc. EtOAc during 1 hr., refrigerated 12 hrs., concentrated to half-volume, diluted to incipient turbidity with Et₂O, and refrigerated several days gave 9.5 g. X, m. 128-35°, Rf 0.95(A). X (4.1 g.) in 30 cc. dioxane treated 3 hrs. with 30 cc. N NaOH, acidified with dilute HCl to pH 2, concentrated, and refrigerated, and the precipitated oil washed with H₂O and repptd. from aqueous EtOH with Et₂O yielded 3.4 g. XII (Z = PhCH₂O₂C) (XIIa), m. 132-40° with sintering (EtOH-H₂O-Et₂O). XIIa (10 g.) in 200 cc. C₆H₆ cleaved in the usual manner with HBr gave 8.25 g. VI 2.HBr (X = CF₃CO, X' = H) (XIII.2HBr), Rf 0.28 (A), 0.65 (B). XIII.2HBr (1 g.) in 20 cc. acetate buffer (pH 4.6) with aqueous Reinecke salt gave the di-reineckate of XIII, red-violet leaflets, m. 140° (decomposition) (H₂O). XIII.2HBr (8.25 g.) in 150 cc. MeCN, 3.15 cc. Et₃N, 9.2 g. PhCH₂ ester (XIV) of IX in 100 cc. MeCN, and 6 g. IV in 50 cc. MeCN yielded in the usual manner 6.55 g. XV (X = CF₃-CO, R = PhCH₂, R' = Et) (XVI), m. 169° with sintering (50% aqueous EtOH), Rf 0.95 (A). XVI (1.13 g.) in 30 cc. MeOH and 30 cc. 0.34N Ba(OH)₂ kept 3 hrs. at room temperature, treated with an equivalent amount N H₂SO₄, filtered, concentrated in vacuo under N to 2 cc., diluted with 20 cc. Me₂CO, and refrigerated several hrs. gave 520 g. XV (X, R, R' = H), amorphous powder, m. 140° with sintering at 80° and gas evolution at 90° (repptd. from H₂O with Me₂CO), Rf 0 (A), 0 (B), 0.4 (80% PhOH). Et lysinate 2HCl (XVII) (2.5 g.) in 50 cc. MeCN, 2.75 cc. Et₃N, 6.6 g. XIV in 50 cc. MeCN, and 5.15 g. IV in 30 cc. MeCN yielded in the usual manner 6.9 g. (crude) XVIII (X = CF₃CO, R = PhCH₂, R' = Et) (XIX), m. 132° with sintering (50% EtOH), Rf 0.9 (A). XIX (4 g.), 75 cc. MeOH, and 75 cc. 0.4N Ba(OH)₂ kept 3 hrs. at room temperature, treated with N H₂SO₄, and worked up in the usual manner yielded 1.4 g. XVIII (X, R, R' = H), microcryst. powder, m. 227° (decomposition) (repptd. from H₂O with Me₂CO), Rf 0.05 (A), 0.00 (B), 0.45 (80% PhOH). XIX (12 g.) stirred 2 hrs. with about 200 cc. dry, Br-free HBr and evaporated yielded 9 g. XVIII (X = CF₃CO, R = H, R' = Et) (XX), Rf

0.8 (A). XX(9 g.) in 100 cc. MeCN adjusted with a few drops Et₃N to pH 3-4, treated with 7.5 g. IV in 20 cc. MeCN and 12.3 g. V in 50 cc. MeCN, and worked up, and the crude product chromatographed on Al₂O₃ yielded 7.1 g. XXI (R = Et, X = CF₃CO, Y = PhCH₂O₂C) (XXII), m. 125-9° with sintering (repptd. from C₆H₆), Rf 0.95 (A). XXII (1.2 g.) in 30 cc. dioxane treated 3 hrs. at room temperature with 30 cc. N NaOH, acidified with dilute HCl to pH 3-4, and concentrated to about 5 cc., and the oily product washed with H₂O and repptd. from EtOH with Et₂O gave an inhomogeneous powder, m. 145-55°; the crude product hydrogenated 6 hrs. in 30 cc. 90% tert-BuOH over Pd black, filtered, and evaporated, and the residue dissolved in 2 cc. H₂O, repptd. with Me₂CO as an oil, redissolved in H₂O, and evaporated over KOH gave 0.29 g. XXI (R, X, Y = H), pale yellow hygroscopic powder, m. 85° with sintering and decomposition at 115°, Rf 0.0 (A), 0.0 (B), 0.6 (80% PhOH). III (14 g.) in 250 cc. EtOAc stirred 5 hrs. with 21 g. p-O₂NC₆H₄OH and 24.5 g. IV, refrigerated overnight, filtered, and evaporated yielded 18.5 g. bis(p-nitrophenyl) ester (XXIII) of III, m. 116° (EtOH). XVII (5.0 g.) in 30 cc. HCONMe₂ and 5.5 cc. Et₃N treated dropwise with stirring during 1 hr. with 10.5 g. XXIII in 20 cc. HCONMe₂, stirred 2 hrs. at room temperature, refrigerated 2 days, concentrated, dissolved in 50 cc. hot Me₂CO, cooled, and filtered, the residue heated 2 hrs. at 50° with 100 cc. 50% aqueous Me₂CO diluted with H₂O to 500 cc., this operation repeated, the mixture filtered, and the crude product ground with 100 cc. MeCN, diluted with 500 cc. H₂O, and filtered off gave 5.8 g. polycondensation product (C₂₁H₂₉N₃O₆)_n, m. 145-60° with sintering; a 5-g. sample extracted 10 hrs. with H₂O in a Soxhlet apparatus, and the extract evaporated gave 1.4 g. product, m. 120-40° with sintering, mol. weight 1100; the undissolved residue was then extracted successively with 500 cc. Me₂CO, EtOH, CHCl₃, and HCONMe₂ each during 10 hrs. each time; each solution was then concentrated and diluted with 10 volume H₂O and the precipitate repptd. from CHCl₃ with Et₂O to yield the following condensation products

(% content in the crude polycondensation product, average mol. weight, m.p., and solvent used are given): 30, 2900, 130-5°, Me₂CO; 22, 3700, 135-8°, EtOH; 5, 4300, 135-40°, CHCl₃; 5, 5500, 135-45°, HCONMe₂. The peptides with free CO₂H and NH₂ groups were subjected in 1% aqueous solution to 5, 10, 20, 30, 45, and 60 hrs. reflux and the cleavage product determined by paper chromatography; the identity of the products is being investigated. The estimation of the amino N by the van Slyke method on all free and some of the protected peptides prepared in this study showed that the γ-carbonamido N is determined only if the α-CO₂H group of the γ-glutamyl group is free.

INDEX TERM: Amides
(poly-, from glutamic acid and lysine)

INDEX TERM: Peptides
(preparation of)

INDEX TERM: Copper, bis[(N6-(dihydrogen N-carboxy-L-γ-glutamyl)-L-lysinate)-, tetrabenzyl ester
Glutamic acid, N-(trifluoroacetyl)-, bis(p-nitrophenyl) ester
Glutamic acid, N-carboxy-, N-benzyl bis(p-nitrophenyl) ester, L-
Lysine, polyamides with L-glutamic acid
Lysine, N₂, N₂'-[N-(trifluoroacetyl)-L-glutamoyl]di-, diethyl ester, dihydrobromide, L-
Lysine, N₂, N₂'-[N-(trifluoroacetyl)-L-glutamoyl]di-, diethyl ester, direineckate, L-
Lysine, N₂, N₂'-[(1-carboxypentamethylene)bis(imino(2-

aminoglutaryl]]di-, dihydrochloride, L-
 Lysine, N2,N2'-[(1-carboxypentamethylene)bis[imino[2-(2,2,2-trifluoroacetamido)glutaryl]]]bis[N6-carboxy-, dibenzyl tri-Et ester, L-
 Lysine, N2,N2'-L-glutamoylbis[N6-carboxy-, dibenzyl ester, hydrochloride, L-
 Lysine, N2,N2'-L-glutamoylbis[N6-L-γ-glutamyl-, L-
 Lysine, N2,N2'-L-glutamoyldi-, diethyl ester, trireineckate, L-
 Lysine, N2,N6-di-L-γ-glutamyl-, L-
 Lysine, N6-(N-carboxy-L-γ-glutamyl)-, dibenzyl ester, Cu complex, L-
 Lysine, N6-(N-carboxy-L-γ-glutamyl)-, dibenzyl ester, L-
 Lysine, N6-L-γ-glutamyl-, hydrochloride, L-

INDEX TERM:

1956-96-3, Lysine, N2, N2'-[N-(trifluoroacetyl)-L-glutamoyl]bis[N6-[N-(trifluoroacetyl)-L-γ-glutamyl]-, dibenzyl di-Et ester, L- 2599-75-9, Lysine, N2,N6-bis[N-(trifluoroacetyl)-L-γ-glutamyl]-, ethyl ester, L- 4627-59-2, Lysine, N2,N6-bis[N-(trifluoroacetyl)-L-γ-glutamyl]-, dibenzyl Et ester, L- 10241-89-1, Lysine, N2, N2'-[N-(trifluoroacetyl)-L-glutamoyl]bis[N6-carboxy-, dibenzyl di-Et ester, L- 17105-15-6, Lysine, N6-L-γ-glutamyl-, L- 96214-20-9, Lysine, N2,N2'-L-glutamoyldi-, diethyl ester, trihydrobromide, L- 106524-30-5, Lysine, N2,N2'-(N-carboxy-L-glutamoyl)bis[N6-carboxy-, tribenzyl di-Et ester, L- 145249-30-5, D-Glutamic acid, polymer with L-lysine (preparation of)

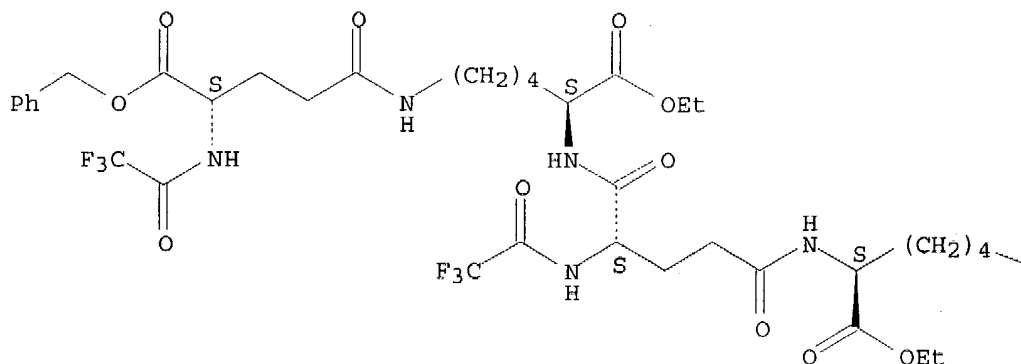
IT 1956-96-3, Lysine, N2, N2'-[N-(trifluoroacetyl)-L-glutamoyl]bis[N6-[N-(trifluoroacetyl)-L-γ-glutamyl]-, dibenzyl di-Et ester, L- (preparation of).

RN 1956-96-3 HCAPLUS

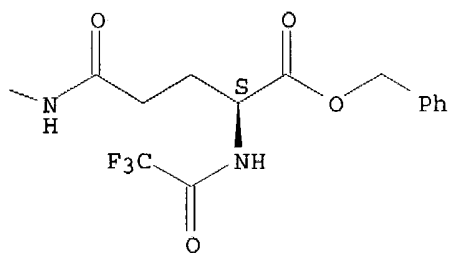
CN Lysine, N2,N2'-[N-(trifluoroacetyl)-L-glutamoyl]bis[N6-[N-(trifluoroacetyl)-L-γ-glutamyl]-, dibenzyl diethyl ester (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



=>

=> diall 6

L24 ANSWER 6 OF 6 CAOLD COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: CA60:657g CAOLD

TITLE: peptides - (XXXV) synthesis of α,ω -oligamides
from L-glutamic acid and L-lysine

AUTHOR NAME: Zahn, Helmut; Paetzold, W.

INDEX TERM: 1683-01-8 1881-71-6 **1956-96-3** 2023-31-6
2599-75-9 4627-59-2 10241-87-9 10241-89-1 17105-15-6
49761-26-4 94429-82-0 94729-49-4 96214-20-9 97255-86-2
97357-55-6 100992-14-1 104377-08-4 105816-73-7
106301-51-3 106524-30-5 106979-36-6 108152-53-0

=> FIL STNGUIDE

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Oct 8, 2004 (20041008/UP).

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FILE RELOADED ON OCTOBER 20, 2002

FILE LAST UPDATED ON JUNE 15, 2004

FILE COVERS 1771 TO 2003.

*** FILE CONTAINS 8,997,153 SUBSTANCES ***

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>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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 * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
 * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
 * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
 * FOR PRICE INFORMATION SEE HELP COST *

NEW

* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
 * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> d que nos 128

L17 STR

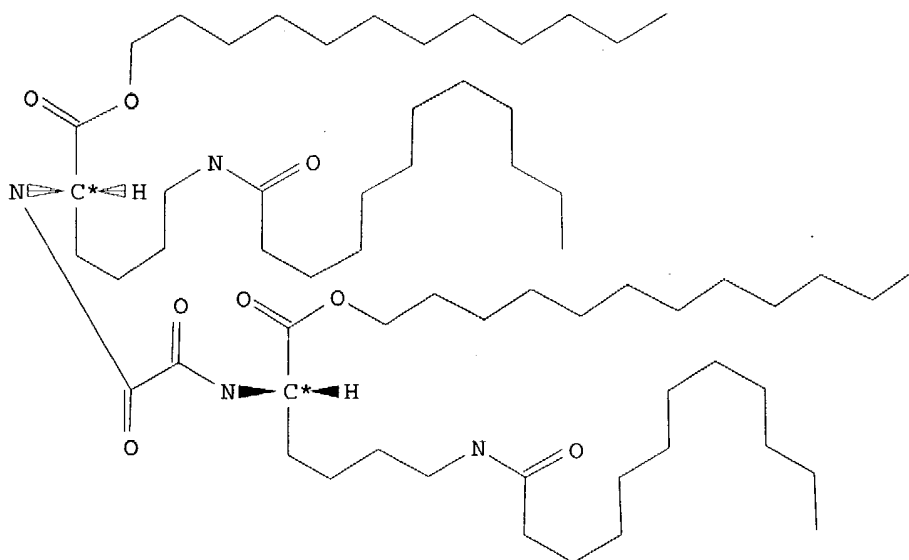
L27 7 SEA FILE=BEILSTEIN SSS FUL L17

L28 7 SEA FILE=BEILSTEIN ABB=ON PLU=ON L27 NOT RN/FA

=> d ide 128 1

L28 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	9609788
Chemical Name (CN):	6-dodecanoylamino-2-<(5-dodecanoylamino-1-dodecyloxycarbonyl-pentylaminooxalyl)-amino>-hexanoic acid dodecyl ester
Autonom Name (AUN):	6-dodecanoylamino-2-<(5-dodecanoylamino-1-dodecyloxycarbonyl-pentylaminooxalyl)-amino>-hexanoic acid dodecyl ester
Molec. Formula (MF):	C62 H118 N4 O8
Molecular Weight (MW):	1047.64
Lawson Number (LN):	3408, 1516, 1237, 380
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	8103123
Tautomer ID (TAUTID):	9010884
Entry Date (DED):	2004/04/23
Update Date (DUPD):	2004/04/23



Field Availability:

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AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx l28 1

L28 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9450810
 Reactant BRN (.RBRN): 9600928, 1361988
 Reactant (.RCT): 2-amino-6-dodecanoylamino-hexanoic acid
 dodecyl ester, oxalyl dichloride

Product BRN (.PBRN): 9609788
Product (.PRO): 6-dodecanoylamino-2-<(5-dodecanoylamino-1-dodecyloxy carbonyl-pentylaminooxalyl)-amino>-hexanoic acid dodecyl ester
No. of React. Details (.NVAR): 1

Reaction Details:

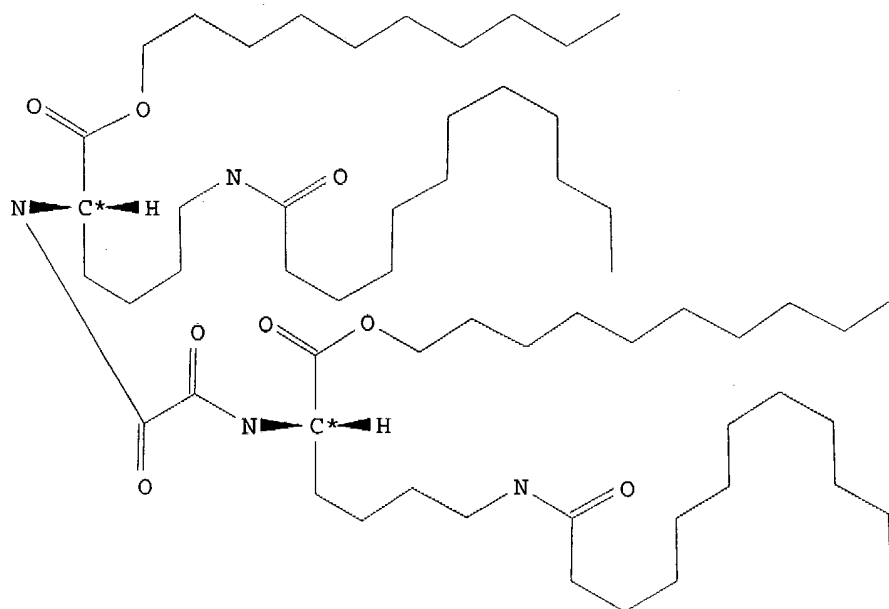
RX

Reaction RID (.RID): 9450810.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): NEt3
Solvent (.SOL): tetrahydrofuran
Time (.TIM): 24 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko; Kimura, Mutsumi; Shirai, Hirofusa; Kenji, Hanabusa, Tetrahedron Lett., CODEN: TELEAY, 44(36), <2003>, 6841 - 6844; BABS-6416910

=> d ide 128 2

L28 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9609441
Chemical Name (CN): 2-<(1-decyloxy carbonyl-5-dodecanoylamino-pentylaminooxalyl)-amino>-6-dodecanoylamino-hexanoic acid decyl ester
Autonom Name (AUN): 2-<(1-decyloxy carbonyl-5-dodecanoylamino-pentylaminooxalyl)-amino>-6-dodecanoylamino-hexanoic acid decyl ester
Molec. Formula (MF): C58 H110 N4 O8
Molecular Weight (MW): 991.53
Lawson Number (LN): 3408, 1516, 1237, 362
File Segment (FS): Stereo compound
Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 8102918
Tautomer ID (TAUTID): 9010610
Entry Date (DED): 2004/04/23
Update Date (DUPD): 2004/04/23



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx 128 2

L28 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9450797
 Reactant BRN (.RBRN): 9455042, 1361988

Reactant (.RCT): Nε-lauroyl-L-lysine decyl ester,
oxalyl dichloride
Product BRN (.PBRN): 9609441
Product (.PRO): 2-<(1-decyloxycarbonyl-5-dodecanoylamino-
pentylaminooxalyl)-amino>-6-
dodecanoylamino-hexanoic acid decyl ester
No. of React. Details (.NVAR): 1

Reaction Details:

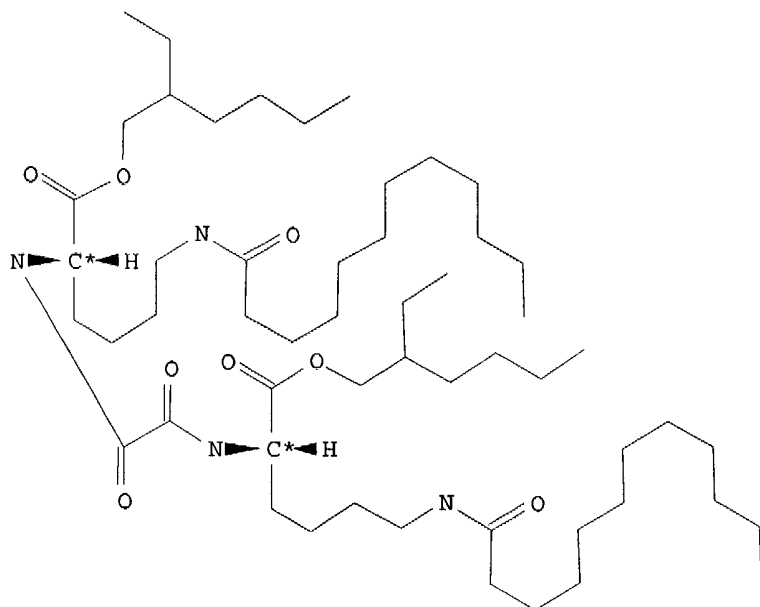
RX

Reaction RID (.RID): 9450797.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): NET3
Solvent (.SOL): tetrahydrofuran
Time (.TIM): 24 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko; Kimura, Mutsumi;
Shirai, Hirofusa; Kenji, Hanabusa, Tetrahedron Lett., CODEN: TELEAY,
44(36), <2003>, 6841 - 6844; BABS-6416910

=> d ide 128 3

L28 ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9608844
Chemical Name (CN): 6-dodecanoylamino-2-<<5-dodecanoylamino-1-
(2-ethyl-hexyloxycarbonyl)-
pentylaminooxalyl>-amino>-hexanoic acid
2-ethyl-hexyl ester
Autonom Name (AUN): 6-dodecanoylamino-2-<<5-dodecanoylamino-1-
(2-ethyl-hexyloxycarbonyl)-
pentylaminooxalyl>-amino>-hexanoic acid
2-ethyl-hexyl ester
Molec. Formula (MF): C54 H102 N4 O8
Molecular Weight (MW): 935.42
Lawson Number (LN): 3408, 1516, 1237, 345
File Segment (FS): Stereo compound
Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 8102462
Tautomer ID (TAUTID): 9010187
Entry Date (DED): 2004/04/23
Update Date (DUPD): 2004/04/23



Field Availability:

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AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx 128 3

L28 ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9450809
 Reactant BRN (.RBRN): 9595999, 1361988

Reactant (.RCT): 2-amino-6-dodecanoylamino-hexanoic acid
2-ethyl-hexyl ester, oxalyl dichloride
Product BRN (.PBRN): 9608844
Product (.PRO): 6-dodecanoylamino-2-<<5-dodecanoylamino-1-
(2-ethyl-hexyloxycarbonyl)-
pentylaminooxalyl>-amino>-hexanoic acid
2-ethyl-hexyl ester
No. of React. Details (.NVAR): 1

Reaction Details:

RX

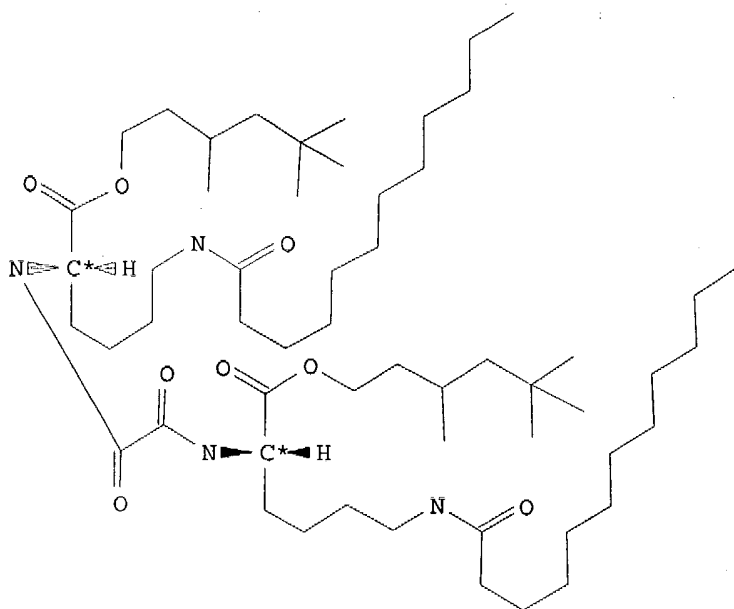
Reaction RID (.RID): 9450809.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): NEt3
Solvent (.SOL): tetrahydrofuran
Time (.TIM): 24 hour(s)
Temperature (.T): 20 Cel
Reference(s):

1. Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko; Kimura, Mutsumi; Shirai, Hirofusa; Kenji, Hanabusa, Tetrahedron Lett., CODEN: TELEAY, 44(36), <2003>, 6841 - 6844; BABS-6416910

=> d ide 128 4

L28 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9608762
Chemical Name (CN): 6-dodecanoylamino-2-<<5-dodecanoylamino-1-
(3,5,5-trimethyl-hexyloxycarbonyl)-
pentylaminooxalyl>-amino>-hexanoic acid
3,5,5-trimethyl-hexyl ester
Autonom Name (AUN): 6-dodecanoylamino-2-<<5-dodecanoylamino-1-
(3,5,5-trimethyl-hexyloxycarbonyl)-
pentylaminooxalyl>-amino>-hexanoic acid
3,5,5-trimethyl-hexyl ester
Molec. Formula (MF): C56 H106 N4 O8
Molecular Weight (MW): 963.48
Lawson Number (LN): 3408, 1516, 1237, 356
File Segment (FS): Stereo compound
Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 8102397
Tautomer ID (TAUTID): 9010090
Entry Date (DED): 2004/04/23
Update Date (DUPD): 2004/04/23



Field Availability:

Code	Name	Occurrence
=====	=====	=====
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx 128 4

L28 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9450808
 Reactant BRN (.RBRN): 9595310, 1361988

Reactant (.RCT): 2-amino-6-dodecanoylamino-hexanoic acid
3,5,5-trimethyl-hexyl ester, oxalyl
dichloride
Product BRN (.PBRN): 9608762
Product (.PRO): 6-dodecanoylamino-2-<<5-dodecanoylamino-1-
(3,5,5-trimethyl-hexyloxycarbonyl)-
pentylaminooxalyl>-amino>-hexanoic acid
3,5,5-trimethyl-hexyl ester
No. of React. Details (.NVAR): 1

Reaction Details:

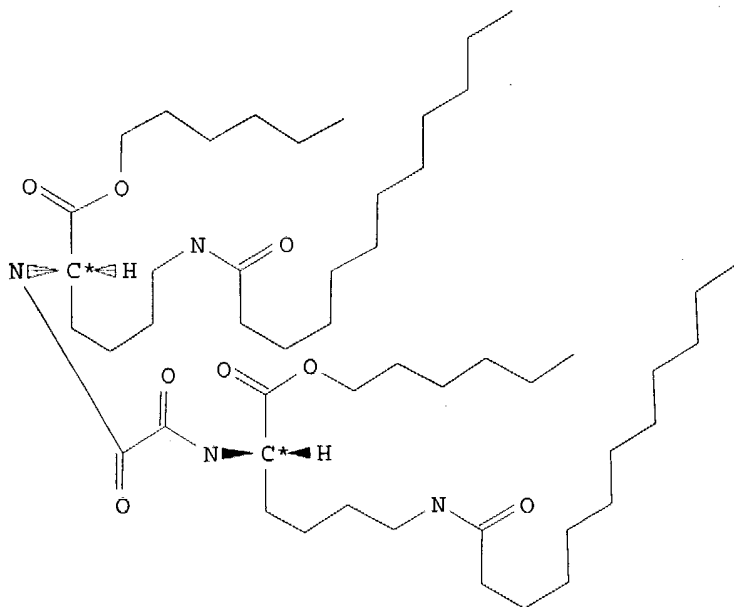
RX

Reaction RID (.RID): 9450808.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): NEt3
Solvent (.SOL): tetrahydrofuran
Time (.TIM): 24 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko; Kimura, Mutsumi;
Shirai, Hirofusa; Kenji, Hanabusa, Tetrahedron Lett., CODEN: TELEAY,
44(36), <2003>, 6841 - 6844; BABS-6416910

=> d ide 128 5

L28 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9608592
Chemical Name (CN): 6-dodecanoylamino-2-<(5-dodecanoylamino-1-
hexyloxycarbonyl-pentylaminooxalyl)-amino>-
hexanoic acid hexyl ester
Autonom Name (AUN): 6-dodecanoylamino-2-<(5-dodecanoylamino-1-
hexyloxycarbonyl-pentylaminooxalyl)-amino>-
hexanoic acid hexyl ester
Molec. Formula (MF): C50 H94 N4 O8
Molecular Weight (MW): 879.31
Lawson Number (LN): 3408, 1516, 1237, 334
File Segment (FS): Stereo compound
Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 8102278
Tautomer ID (TAUTID): 9009997
Entry Date (DED): 2004/04/23
Update Date (DUPD): 2004/04/23



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
FBRN	Fragment BRN	2
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx 128 5

L28 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX

Reaction ID (.ID): 9450806
Reactant BRN (.RBRN): 9593967, 1361988
Reactant (.RCT): 2-amino-6-dodecanoylamino-hexanoic acid
hexyl ester, oxalyl dichloride
Product BRN (.PBRN): 9608592
Product (.PRO): 6-dodecanoylamino-2-<(5-dodecanoylamino-1-
hexyloxycarbonyl-pentylaminooxalyl)-amino>-
hexanoic acid hexyl ester
No. of React. Details (.NVAR): 1

Reaction Details:

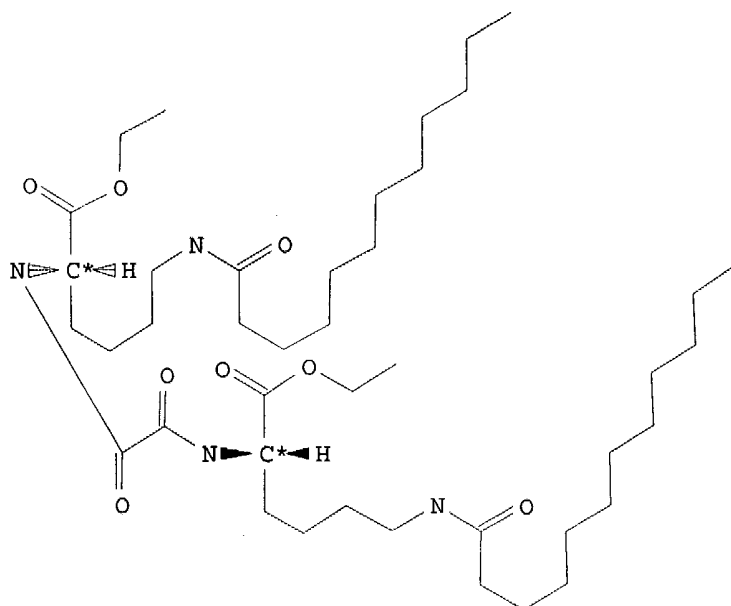
RX

Reaction RID (.RID): 9450806.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): NEt3
Solvent (.SOL): tetrahydrofuran
Time (.TIM): 24 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko; Kimura, Mutsumi;
Shirai, Hirofusa; Kenji, Hanabusa, Tetrahedron Lett., CODEN: TELEAY,
44(36), <2003>, 6841 - 6844; BABS-6416910

=> d ide 128 6

L28 ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9607318
Chemical Name (CN): 6-dodecanoylamino-2-<(5-dodecanoylamino-1-
ethoxycarbonyl-pentylaminooxalyl)-amino>-
hexanoic acid ethyl ester
Autonom Name (AUN): 6-dodecanoylamino-2-<(5-dodecanoylamino-1-
ethoxycarbonyl-pentylaminooxalyl)-amino>-
hexanoic acid ethyl ester
Molec. Formula (MF): C42 H78 N4 O8
Molecular Weight (MW): 767.10
Lawson Number (LN): 3408, 1516, 1237, 298
File Segment (FS): Stereo compound
Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 8101228
Tautomer ID (TAUTID): 9009109
Entry Date (DED): 2004/04/23
Update Date (DUPD): 2004/04/23



Field Availability:

Code	Name	Occurrence
=====	=====	=====
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	4
NMR	Nuclear Magnetic Resonance	4

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=====	=====	=====
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx 128 6

L28 ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9450796
Reactant BRN (.RBRN): 8726560, 1361988
Reactant (.RCT): Nε-lauroyl-L-lysine ethyl ester,
oxalyl dichloride
Product BRN (.PBRN): 9607318
Product (.PRO): 6-dodecanoylamino-2-<(5-dodecanoylamino-1-
ethoxycarbonyl-pentylaminooxalyl)-amino>-
hexanoic acid ethyl ester
No. of React. Details (.NVAR): 1

Reaction Details:

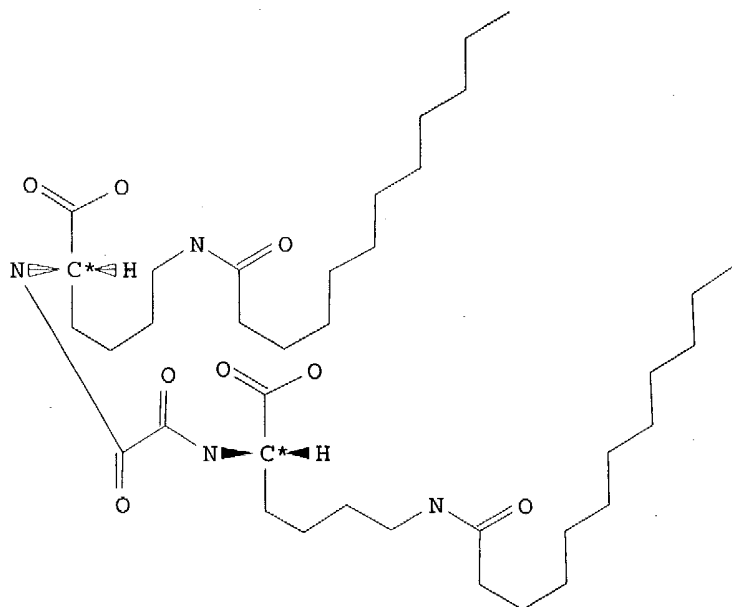
RX

Reaction RID (.RID): 9450796.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): NEt3
Solvent (.SOL): tetrahydrofuran
Time (.TIM): 24 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko; Kimura, Mutsumi;
Shirai, Hirofusa; Kenji, Hanabusa, Tetrahedron Lett., CODEN: TELEAY,
44(36), <2003>, 6841 - 6844; BABS-6416910

=> d ide 128 7

L28 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9606932
Chemical Name (CN): 2-<(1-carboxy-5-dodecanoylamino-
pentylaminooxalyl)-amino>-6-
dodecanoylamino-hexanoic acid
Autonom Name (AUN): 2-<(1-carboxy-5-dodecanoylamino-
pentylaminooxalyl)-amino>-6-
dodecanoylamino-hexanoic acid
Molec. Formula (MF): C38 H70 N4 O8
Molecular Weight (MW): 710.99
Lawson Number (LN): 3408, 1516, 1237
File Segment (FS): Stereo compound
Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 8100911
Tautomer ID (TAUTID): 9008795
Entry Date (DED): 2004/04/23
Update Date (DUPD): 2004/04/23



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d rx 128 7

L28 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9450793
 Reactant BRN (.RBRN): 6928812, 1361988

Reactant (.RCT): Nε-lauroyl-L-lysine, oxalyl
dichloride
Product BRN (.PBRN): 9606932
Product (.PRO): 2-<(1-carboxy-5-dodecanoylamino-
pentylaminooxalyl)-amino>-6-
dodecanoylamino-hexanoic acid
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 9450793.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 79 percent (BRN=9606932)
Reagent (.RGT): aq. NaOH
Solvent (.SOL): diethyl ether
Time (.TIM): 23 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Suzuki, Masahiro; Nigawara, Tomomi; Yumoto, Mariko; Kimura, Mutsumi;
Shirai, Hirofusa; Kenji, Hanabusa, Tetrahedron Lett., CODEN: TELEAY,
44(36), <2003>, 6841 - 6844; BABS-6416910

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